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4A.3 A CFD MODEL INTERCOMPARISON AND VALIDATION USING HIGH RESOLUTION WIND TUNNEL DATA

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1. INTRODUCTION

Aggressive model development has been underway at Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL) in order to meet the exterior modeling requirements of the Department of Energy Chemical and Biological Weapons Nonproliferation Program (DOE CBNP). This development effort has been directed in two main areas. The first has been the extension of modeling capabilities by adding improved numerical schemes, and code modifications to take advantage of massively parallel architectures and nesting. The second has been the improvement and/or development and testing of physical parameterizations for surface effects (e.g., thermal, wall effects, canopy), turbulence, and chemistry (for instance deposition, degradation of chemical species). These efforts will ultimately give DOE the capability to incorporate the results of high quality, multiscale computational fluid dynamics (CFD) simulations at a wide range of resolutions from 1 m (one to several resolved buildings) to over 100 m (tens to hundreds of buildings) into its overall planning and response capability for releases of hazardous agents.

One important aspect of the DOE CBNP exterior modeling program is the validation of these CFD models using available data from a number of sources, including wind tunnel studies and upcoming field studies. This paper reports some preliminary comparisons of model simulations with data obtained from the U. S. Environmental Protection Agency Fluid Modeling Facility (USEPA FMP) for the mean and turbulent components of the flow field around a 2-D array of model buildings.

2. MODELS

Two CFD models are being used as platforms to develop this overall modeling capability. HIGRAD is a model that has been under development as part of collaborative modeling effort between Los Alamos National Laboratory and NCAR (National Center for Atmospheric Research). FEM3MP is the result of several years of research at LLNL involving advanced turbulence models and finite element methods (Gresho and Chan, 1998, Stevens et al. 1999).

HIGRAD solves the three dimensional Navier Stokes equations in a terrain-following coordinate system. The model is second-order accurate, and uses a non-oscillatory forward in time advection scheme that can accurately model regions of strong shear (Smolarkiewicz and Grabowsky, 1990; Smolarkiewicz and Margolin, 1993; Smolarkeiwicz and Margolin, 1994). A Smagorinsky-type and TKE-based large eddy simulation (LES) turbulence closure have been incorporated into the code. HIGRAD has been modified to allow for the computation of flow around buildings. The model can be run in an anelastic mode, using an efficient conjugate residual pressure solver (Smolarkiewicz and Margolin, 1994), or in a compressible mode using the method of averages (Reisner, 1999). This model has been used in a number of previous studies involving simulation of the convective boundary layer in the tropical atmosphere, and simulation of the diurnal variability of heat and moisture in a riparian environment. As part of the model development efforts at Los Alamos, HIGRAD has also been used for studies of tracer dispersion and transport in an urban area and around the Salt Lake City Delta Center, and to investigate the effect of radiative heating and shading on the flow field and tracer transport around buildings (Reisner et al., 1998; Smith and Reisner, 1999, Decroix et al., 2000).

FEM3CB and FEM3MP also solve the three dimensional Navier-Stokes equations. These models use a finite element discretization that is

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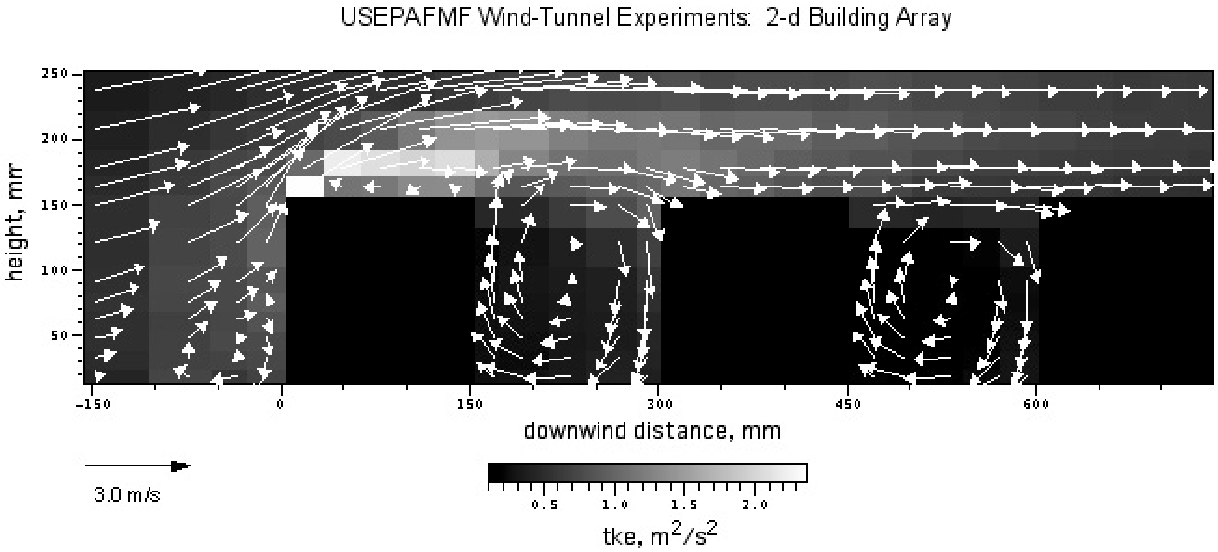

Figure 1. Mean wind vectors and TKE field measured along centerline around the 2-D building array in the USEPA wind tunnel. The first three of seven buildings are shown. (From Brown et al., 2000, this issue)

capable of representing a very complex urban geometry with O(100) buildings embedded in the mesh. FEM3CB is the most recent version of the model FEM3C that was originally developed to handle the flow and dispersion of heavier than air gases (Chan and Lee, 1999). FEM3CB uses an anelastic approximation and an implicit time discretization that allows fo a wide range of stability conditions to be simulated and for larger time steps to be taken, respectively. FEM3MP, the emerging replacement of FEM3CB, has been ported to several parallel platforms and incorporates an advanced multigrid Poisson solver (Stevens et al., 1999). These models contain several turbulence closures that make them uniquely suited to investigating the use of CFD for the simulation of flow and dispersion around buildings. The two principle turbulence models are a LES subgrid model (Smagorinsky, 1963) with a treatment of boundary surface taken from Mason, 1994, and a three-equation RANS model. The RANS results presented here are from FEM3CB.

3. WIND TUNNEL DATA

Model validation runs used data obtained from a recent USEPA wind tunnel study of the flow field around a 2-D array of model buildings consisting of seven evenly spaced rectangular blocks of equal height (H_b) and longitudinal length 0.15 m. In this study, the spacing between each building row was 1.0 H_b, and the building rows spanned the horizontal extent of the wind tunnel. A neutral atmospheric boundary layer was simulated in the wind tunnel using spires and floor roughness elements upstream of the 2-D building array. High-resolution measurements of the three components of mean and turbulent velocity statistics were taken with a pulsed wire anemometer at various heights within each canyon, above each building, and upstream and downstream of the building array. These measurements were taken at a rate of 10 Hz and averaged over a period of 120 s. A detailed description of the wind tunnel experimental setup and results is presented in Brown et al. (2000) (this conference).

Figure 1 shows a crossection down the longitudinal centerline of the observed turbulent kinetic energy (TKE) and mean wind vectors, which reveal the overall flow pattern. The figure shows a flow separation and corresponding recirculation over the first building rooftop. There is no similar recirculation over the other buildings. There are well-developed clockwise rotating vortices in each of the canyons. TKE peaks at the upwind edge of the first building. TKE values are also largest above the canyons.

4. MODEL VALIDATION

Model validation efforts using the USEPA data are currently in progress at LANL and LLNL. These efforts are designed to identify and improve model parameterizations, numerical procedures, and methods of model initialization, as well as to document the performance of the

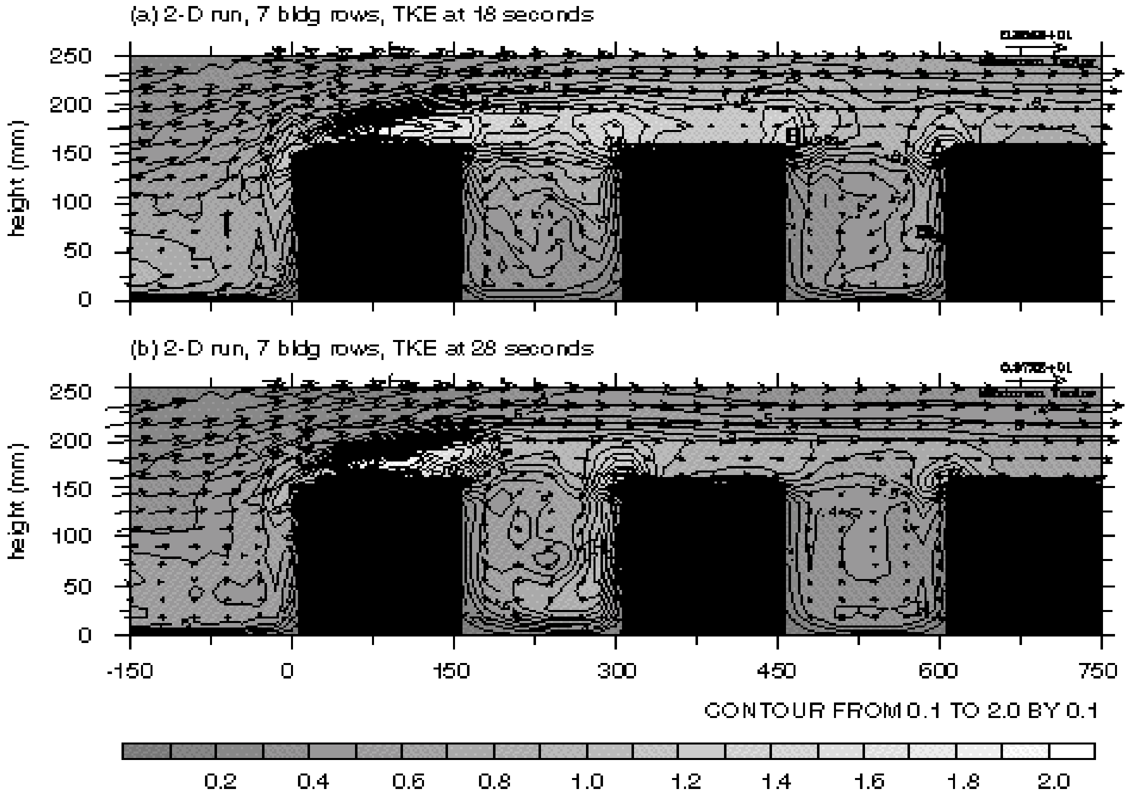

Figure 2. Instantanous wind vectors and TKE field computed by LES model at (a) 18 s, (b) 28 s showing flow reversal in first canyon. First three buildings are shown.

models. The validation of these models against controlled experiments is particularly valuable given the wide variety of factors influencing simulations of flow around complex urban geometries. Physical processes such as surface heating and microphysical effects can cause important convective effects (Smith and Reisner, 1999). Numerics are also important. FEM3CB uses a non-dissipative finite element transport algorithm, whereas HIGRAD uses a dissipative monotonic scheme. The former model is better at preserving energies, the latter at minimizing nonphysical extrema. The role of total explicit and implicit dissipation in monotonic simulations of turbulence is still unknown. The choice of turbulence model can also affect the total amount of dissipation. This can dramatically affect results of numerical simulations. Finally, uncertainty in the initialization of flows, the type of boundary conditions used, and the ability to faithfully represent the geometry of the underlying topography and buildings are important factors. Conducting validation studies that compare high quality experimental data will do much to establish answers to these questions. In this text, we will consider the role of steady state turbulence modeling and that of 2-D versus 3-D modeling.

One fundamental issue is the role of the turbulence closure in the simulation. Two fundamental types of models are RANS and LES modeling. The turbulence closure is a model independent issue as both models are capable of this type of simulation merely by altering the turbulence module used. One conclusion that is often neglected by LES models, especially in shear driven flows such as this one, is that LES often requires an order of magnitude more computer resources for a given level of accuracy than a RANS simulation. Implicit in the LES assumption is that the mesh and time step can capture all of the temporal and spatial organization of the flow, whereas for RANS, much larger space and time scales are incorporated analytically into the model. In RANS models, fewer time steps are required, since most of the turbulent scales are parameterized and one is usually interested in convergence toward a steady state. Therefore, there is no need to capture the minimum of

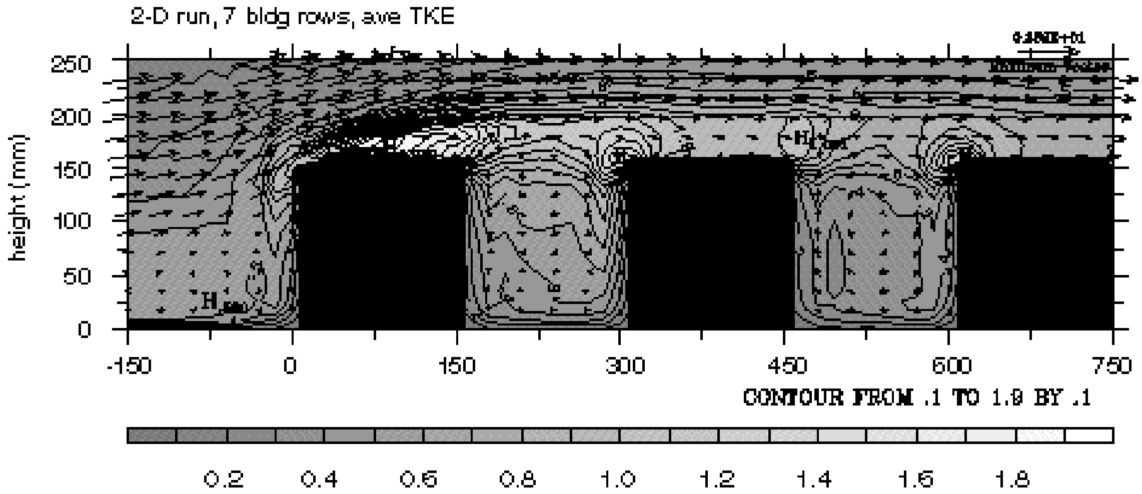

Figure 3. LES modeled mean wind vectors and TKE field. First three buildings are shown.

5~10 eddy turnovers needed for useful statistical averaging. The need for these extra resources is often seen in cases where, for a coarse resolution, LES is less accurate than RANS. In these cases, the LES turbulence closure is forced to handle much larger eddy scales than it is designed for. Therefore, the LES coarse grid solution in effect becomes a RANS with a crude turbulence model. One question that is being investigated is the level of resolution required for LES to surpass RANS modeling. Also, is the numerical expense of LES cost effective or is that answer dependent on the purpose of the simulation? It must be stated that LES offers additional temporal quantities such as resolved variances and concentration fluctuations, which are unavailable in a RANS simulation.

4. RESULTS

This paper shows preliminary validation results for LES (HIGRAD) and RANS (FEM3CB) simulations. Both 2-D and 3-D simulations are being performed. Only results of the 2-D LES simulations are shown here. For the LES runs, the domain size for model simulations shown was 5.4 m in the longitudinal direction and 1.4 m in the vertical direction. The domain consisted of 360x1x51 grids. The resolution in the longitudinal direction was 0.015 m. The vertical spacing was 0.05 H_b near the surface, and increased to 0.1 H_b near the top of the model domain. The inflow profile for the mean velocity was determined from the wind tunnel data. The simulations were conducted for a time span of one minute with a time increment of 0.001 s. The model incorporates sub-grid scale turbulence closure using the Smagorinsky parameterization (Smagorinsky 1963), and a standard "law-of-wall" parameterization is used for the ground and building surfaces to account for momentum fluxes near the surfaces. However, the use of a sub-grid scale turbulence closure at the small scale of these simulations resulted in an excessively large recirculation over the first building that extended beyond the first building. This resulted in a canyon recirculation that was counter to the wind tunnel observed recirculation. This feature was seen in both the LANL and LLNL LES model simulations and needs further investigation. We found that excluding any subgrid turbulence closure for these runs yielded better results.

Figures 2a and 2b illustrate the usefulness of LES in simulating the time varying flow field. Figure 2a shows a snapshot of the vertical crossection of TKE and velocity vectors at 18 s. Figure 2b shows a similar snapshot at 28 s. Figure 2b shows a clockwise rotation in the first canyon, while Fig. 2a shows a reverse recirculation. On average, the recirculation in all canyons is clockwise, but due to the turbulent nature of the flow in and above the canyons, this flow occasionally reverses as seen in Fig. 2b. This behavior was also seen in smoke visualizations in the wind tunnel study.

Figure 3 shows a vertical cross section of the modeled TKE and mean velocity vectors. Figure 1 shows the corresponding TKE crossection from the wind-tunnel study. Local maxima for the turbulence fields in the vicinity of the upstream

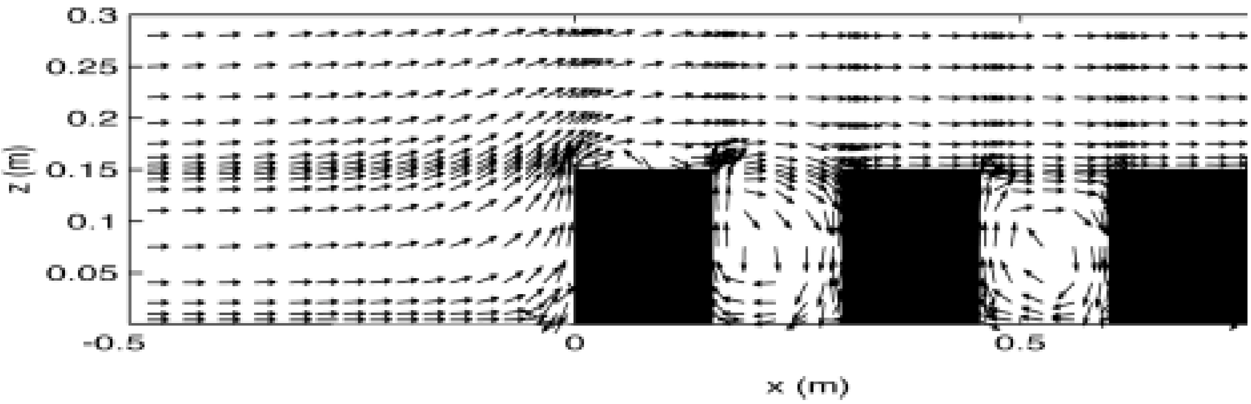

Figure 4. RANS modeled wind vectors (normalized) around 2-D building array. First three buildings are shown.

corners of each building are also evident in both model computations and measurements. Interestingly, the modeled TKE is similar to the observed TKE in pattern and magnitude despite the 2-D nature of the simulation.

The modeled flow field matches the wind-tunnel observations reasonably well. For example, a small recirculation zone upstream of the first building is simulated, as observed in the wind tunnel study. The model simulation also reproduces the flow separation and recirculation at the top of the first building. These features are not evident for the other buildings. Well-defined clockwise rotation in the canyons is also evident for the model simulation and wind-tunnel observations. The cavity flow downstream of the building array is also well represented by the model.

The RANS approach in FEM3CB uses a three equation model. It is an improvement on k-ε modeling with the effective addition of a third quantity, the second invariant of the anisotropic part of the Reynolds Stress tensor. By using this additional equation, one is able to incorporate many of the characteristics of second-order closure into the turbulence model. This is a considerably more accurate approach than that of simple down-gradient diffusion. A relatively coarse mesh of 167 elements was used in the stream wise direction, 26 in the vertical, and 15 in the span wise. The domain dimensions were respectively 3.0 meters long, 0.5 m high, and 1.5 m deep.

Figure 4 shows normalized wind vectors around the first three buildings. These vectors have been normalized to give each vector an equal length and are used to show vector orientation. Although the results are preliminary, they appear to agree well with observations, in that all of the flow features observed are present in the simulation with velocities that are similar in magnitude (not shown). In Fig. 5, streamlines of the flow are shown. Before the first block, a small recirculating eddy is seen at its base. The recirculating eddy at the top of the first block does not block the flow past the entrance to the first cavity. This results in a clockwise vortex in each of the cavities between the blocks. In the third cavity, there is a classical lid driven cavity flow with the vortex being shifted to the upper right hand corner of the cavity. For relatively coarse resolution, a high quality simulation has been performed. It is projected that this simulation in FEM3MP could be performed in under half an hour using massively parallel computing platforms. This makes RANS modeling a powerful assessment tool for quickly examining a large number of scenarios.

6. CONCLUSIONS

Model validation efforts using USEPA data are currently in progress at LANL and LLNL in order to meet the exterior modeling requirements of the DOE CBNP program. Initial model validation results for both LES and RANS based simulations show reasonable agreement with wind-tunnel data. Major features such as the flow separation and recirculation at the upwind edge of the first model building, and clockwise vortices in the canyons are reasonably well reproduced using both LES and RANS turbulence closures. The LES is able to show the time-varying nature of the flow field, especially in the canyons and downstream of the building array. The RANS simulation achieved comparable results for mean fields at far less computational cost.

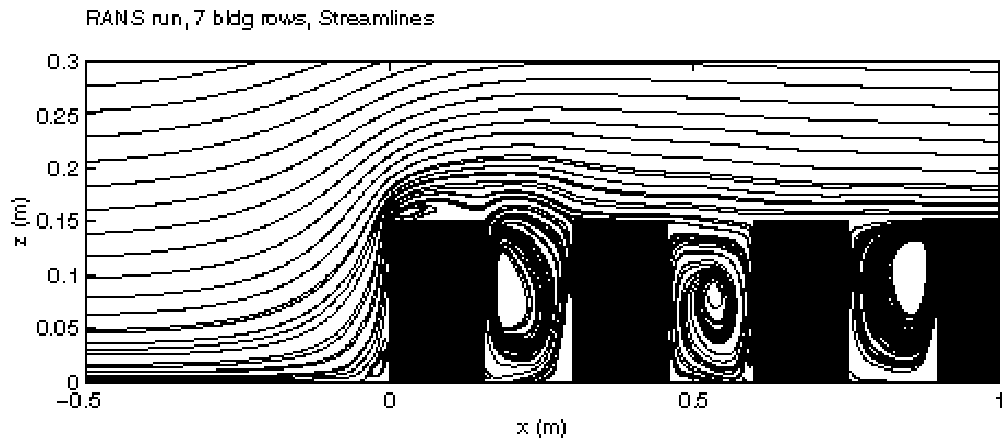

Figure 5. Streamlines of RANS simulated flow around 2-D building array. First four buildings are shown.

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